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MIXED LIGAND COORDINATION COMPOUNDS OF CALCIUM ACETATE WITH SOME ORGANIC LIGANDS

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ABSTRACT

Mixed-ligand coordination compounds of calcium acetate have been synthesized. The composition, identity, methods of coordination of acetate groups, molecules of formamide, acetamide, carbamide, thiocarbamide have been established, and the thermal behavior of the obtained complexes has been studied.

KEYWORDS

Mixed-ligand coordination compounds, organic ligands, formamide, acetamide, urea, thiourea.

Introduction

Molecules of formamide (FA), acetamide (AA), urea (U), thiourea (TU) and acetic acid anion contain donor atoms and promote the formation of coordination compounds with metal ions. In [1-3], coordination compounds of a number of metal carboxylates with amides were synthesized and studied. There are no data on mixed-ligand coordination compounds of calcium acetate in the scientific literature.

To carry out the synthesis of coordination compounds, we have chosen the most efficient mechanochemical method, since it does not require scarce organic solvents. The synthesis procedure was carried out according to [4, 5]. Complex compounds $Ca(CH_3COO)_2 \cdot 2FA \cdot H_2O$, $Ca(CH_3COO)_2 \cdot FA \cdot AA \cdot 2H_2O$, $Ca(CH_3COO)_2 \cdot FA \cdot U \cdot 0.5H_2O$, $Ca(CH_3COO)_2 \cdot FA \cdot TU \cdot 2/3H_2O$ obtained by intensive stirring in an agate mortar for 3 hours 0.01 mol of calcium acetate with 0.02 mol of formamide, 0.01 mol of calcium acetate with 0.01 mol of formamide and 0.01 mol of acetamide, 0.01 mol of acetate calcium with 0.01 mole of formamide and 0.01 mole of urea, 0.01 mole of calcium acetate with 0.01 mole of formamide and 0.01 mole of thiourea.

The synthesized compounds were analyzed for calcium content according to [1-3]. Nitrogen was determined by the Dumas method [1-2], carbon and hydrogen were determined by combustion in an oxygen flow [Table 1]. To establish the individuality of the synthesized compounds, X-ray diffraction patterns were taken on a DRON-2.0 setup with a Cu anticathode [5]. IR absorption spectra were recorded in the region of 400-4000 cm^{-1} on AVATAP-360 spectrometer manufactured by Nicolet [Fig. 1].

Thermal analysis was carried out on F-Paulik-J.Paulik-L.Erdey derivatograph system [6] at a rate of 9 deg/min and a weight of ~0.2 g at a sensitivity of T-900, TG-200, DTA, DTG galvanometers - 1/10. Recording was carried out under atmospheric conditions. A corundum crucible 10 mm in diameter without a lid served as a holder. Al_2O_3 was used as a control.

Comparison of interplanar distances and relative intensities of calcium acetate, acetamide, carbamide (urea), thiocarbamide (tiourea) and complexes based on them showed that the new coordination compounds differ from each other, as well as from the original components, therefore, the compounds have an individual crystal lattice.

Table 1. Results of elemental analysis of mixed-ligand coordination compounds calcium acetate

Compounds	Ca, %		N, %		S, %		C, %		H, %	
	Find.	calc.	Find.	calc.	Find.	calc.	Find.	calc.	Find.	calc.
$Ca(CH_3COO)_2\cdot$ $\cdot 2FA\cdot H_2O$	14,96	15,04	10,39	10,52	-	-	26,88	27,07	5,24	5,30
$Ca(CH_3COO)_2\cdot$ $\cdot FA\cdot AA\cdot 2H_2O$	13,51	13,39	9,43	9,36	-	-	27,89	28,10	5,97	6,06
$Ca(CH_3COO)_2\cdot FA\cdot$ $\cdot U\cdot 0{,}5H_2O$	14,81	14,68	15,51	15,44	-	-	26,41	26,47	5,24	5,18
$Ca(CH_3COO)_2\cdot FA\cdot$ $\cdot TU\cdot 2/3H_2O$	13,69	13,75	14,36	14,43	10,93	11,01	24,68	24,74	5,04	4,96

Frequencies (cm^{-1}) at 3390, 3317-ν (NH_2), 3194-2δ (NH_2), 2888-ν (CH), 1709-ν (CO), 1615-δ (NH_2), 1391-δ (CH), 1316-ν (CN), 1052-r (NH_2), 604-δ (OCN).

IR spectrum of distribution of free acetamide molecules by mass bands at 3378-ν (NH_2), 3199-2δ (NH_2), 1664-ν (CO), 1614-δ(NH_2), ν (CO), 1395-ν (CN), 1352-δ (CH_3), 1148-ρ (NH_2), 1047-ρ (CH_3), 1005-ν (CC), 575-δ (NCO) and 462-δ (CCN).

In the IR absorption spectrum of a free urea molecule, frequencies were found at 3443- νas (NH_2), 3347- νs (NH_2), 3255- 2δ (NH_2), 1679- ν (CO), δ (NH_2), 1624- δ (NH_2), ν (CO), 1464- ν (CN), 1152- , 1057- ρ (NH_2), 1002- ν (CN), 789- δ (NH_2), 573- δ (NCO) and 559- δ (NCN).

The IR absorption spectrum of an uncoordinated thiocarbamide molecule has frequencies at 3380- νas (NH_2), 3276- νs (NH_2), 3178-2δ (NH_2), 1619- δ (NH_2), δ (HNC), 1474- ν (CN), 1413- ν (CS), 1084- ν (CN), 783- ρ (NH_2), 730- ν (CS), 631- δ (CS), δ (NCS), 487- δ (NCN) and 413- δ (NCS).

In the IR absorption spectrum of a free nicotinamide molecule, frequencies were found at 3366- ν (NH2), 3159- 2δ (NH2) 2, 3059- ν (CH), 1681- ν (CO), 1619- δ (NH_2), 1593- νk, 1486, 1423- νk, δ (CNN), 1395-, 1340- ν (CH), δ (CCN), 1202- δ (CCN), 1154, 1124- ν (NH_2), δ (CCN), 1091 - δ (CCN), ν (CO), νk, 1029- νk, δ (CCN), 970- ν (CC), 829- ν (CC), δ (CCC), 778, 703- δ (CCN), δ(CO), 624, 603-δ(CO), δ(CNC), 510-δ(CO), δ(CCC).

An analysis of the IR absorption spectra of non-coordinated molecules of formamide, acetamide, urea and their complex compounds with calcium acetates showed that with the transition to coordinated positions, the values of some frequencies of amide molecules change significantly. Due to the complexity of the IR absorption spectra of complex compounds of calcium acetate with amides, we were unable to attribute all the observed frequencies to the corresponding vibrations of the bond groups. In the formamide complex compound of calcium acetate, the frequencies of the predominant stretching vibration of the C=O bond appear at 1692 cm^{-1}. In mixed compounds

$Ca(CH_3COO)_2 \cdot FA \cdot AA \cdot 2H_2O$ and $Ca(CH_3COO)_2 \cdot FA \cdot K \cdot \cdot 0.5H_2O$, the frequency ν (C=O) appears as total bands at 1673 and 1678 cm^{-1}. While the frequencies of stretching vibrations of the C-N bond for formamide, acetamide and carbamide compounds increase by 32-65, 2 and 36 cm^{-1}, respectively. In the mixed complex $Ca(CH_3COO)_2 \cdot FA \cdot TK \cdot 2/3H_2O$, the frequencies of the C=O and CN bonds of formamide appear at 1693 and 1348 cm-1. In the IR absorption spectrum of an uncoordinated formamide molecule, frequencies (cm-1) were found at 3390, 3317- ν (NH2), 3194- 2δ (NH2), 2888- ν (CH), 1709- ν (CO), 1615-δ (NH2), 1391-δ (CH), 1316-ν (CN), 1052-r (NH2), 604-δ (OCN).

The IR absorption spectrum of a free acetamide molecule is characterized by bands at 3378- ν (NH_2), 3199- 2δ (NH_2), 1664- ν (CO), 1614- δ (NH_2), ν (CO), 1395- ν (CN), 1352-δ(CH_3), 1148-ρ(NH_2), 1047-ρ(CH_3), 1005-ν(CC), 575-δ(NCO) and 462-δ(CCN).

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The IR absorption spectrum of an uncoordinated thiourea molecule has frequencies at 3380- νas (NH_2), 3276- νs (NH_2), 3178-2δ (NH_2), 1619- δ (NH_2), δ (HNC), 1474- ν (CN), 1413- ν (CS), 1084- ν (CN), 783- ρ (NH_2), 730- ν (CS), 631- δ (CS), δ (NCS), 487- δ (NCN) and 413- δ (NCS).

In the IR absorption spectrum of a free nicotinamide molecule, frequencies were found at 3366- ν (NH_2), 3159- 2δ (NH_2), 3059- ν (CH), 1681- ν (CO), 1619- δ (NH_2), 1593- νk, 1486, 1423- νk, δ (CNN), 1395-, 1340- ν (CH), δ (CCN), 1202- δ (CCN), 1154, 1124- ν (NH_2), δ (CCN), 1091 - δ (CCN), ν (CO), νk, 1029- νk, δ (CCN), 970- ν (CC), 829- ν (CC), δ (CCC), 778, 703- δ (CCN), δ(CO), 624, 603-δ(CO), δ(CNC), 510-δ(CO), δ(CCC).

An analysis of the IR absorption spectra of non-coordinated molecules of formamide, acetamide, urea and their complex compounds with calcium acetates showed that with the transition to coordinated positions, the values of some frequencies of amide molecules change significantly. Due to the complexity of the IR absorption spectra of complex compounds of calcium acetate with amides, we were unable to attribute all the observed frequencies to the corresponding vibrations of the bond groups. In the formamide complex compound of calcium acetate, the frequencies of the predominant stretching vibration of the C=O bond appear at 1692 cm^{-1}. In mixed compounds $Ca(CH_3COO)_2 \cdot FA \cdot AA \cdot 2H_2O$ and $Ca(CH_3COO)_2 \cdot FA \cdot K \cdot 0.5H \cdot O$, the frequency ν (C=O) appears as total bands at 1673 and 1678 cm^{-1}. While the frequencies of stretching vibrations of the C-N bond for formamide, acetamide and carbamide compounds increase by 32-65, 2 and 36 cm^{-1}, respectively. In the mixed complex $Ca(CH_3COO)_2 \cdot FA \cdot TK \cdot 2/3H_2O$, the frequencies of the C=O and CN bonds of formamide appear at 1693 and 1348 cm^{-1}. In the low-frequency region of the spectrum, the frequencies of thiocarbamide molecules at 730 and 631 cm^{-1} decrease by 30 and 10 cm^{-1} in the case of the complex. In the low-frequency region of the spectrum, the frequencies of thiocarbamide molecules at 730 and 631 cm^{-1} decrease by 30 and 10 cm^{-1} in the case of the complex. The found changes in the spectrum can be explained by the coordination of the thiocarbamide molecule with the calcium ion through the sulfur atom.

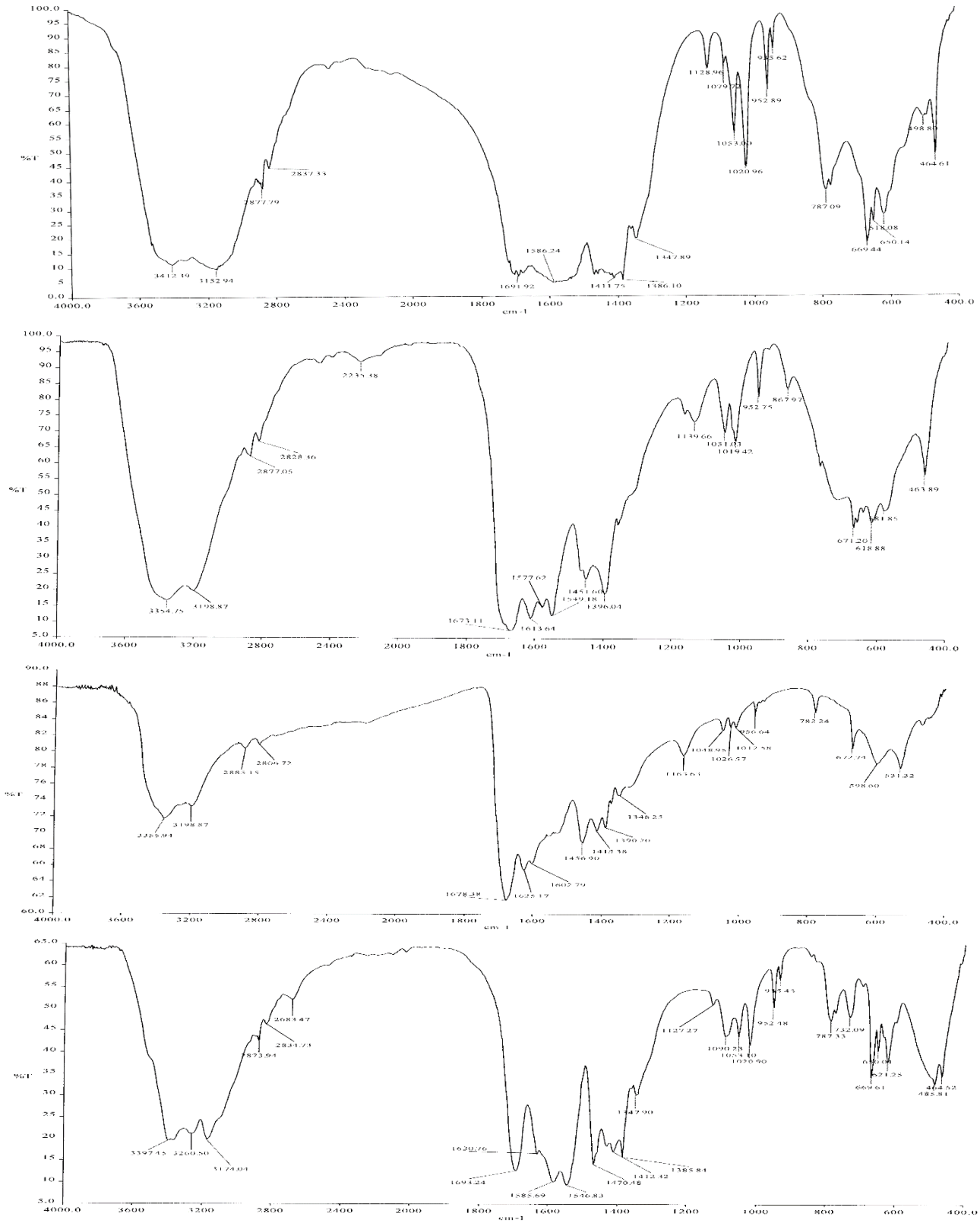

Fig. 1. IR absorption spectra: a - $Ca(CH_3COO)_2 \cdot 2FA \cdot H_2O$, b - $Ca(CH_3COO)_2 \cdot FA \cdot AA \cdot 2H_2O$, c - $Ca(CH_3COO)_2 \cdot FA \cdot K \cdot 0.5H_2O$ and d - $Ca(CH_3COO)_2 \cdot FA \cdot TK \cdot 2/3H_2O$.

The value of the frequency difference νas (COO)- νs (COO) of all compounds is less than 150 cm^{-1}, which corresponds to the bidentate-cyclic coordination of the acetate fragment. In complex compounds, the central ion has a six-coordination site. Water molecules are held together by hydrogen bonds. The thermal study of the synthesized complex compounds showed that the DTA curves of the derivatograms revealed endothermic effects corresponding to the removal and decomposition of bound and coordinated molecules of water, formamide, acetamide, urea, and thiourea, as well as exothermic effects due to the destruction of acetate fragments, combustion of thermal decomposition products, and oxide formation or calcium sulfide.

REFERENCES

1. Ulugbekovich, T. J., Pulatovna, N. K., Aslanbekovich, I. A., & Mamajonovna, T. F. (2023). Coordination Compounds Of Calcium Acetate With Some Ligands. Texas Journal of Engineering and Technology, 18, 12-18.
2. Ulugbekovich, T. J., & Pulatovna, N. K. ELECTRONIC STRUCTURES AND REACTIVITY OF EIGHT MIXED-LIGAND COMPLEXES OF CALCIUM ACETATE BY A QUANTUM-CHEMICAL METHOD. HOMO, 10(9,655), 8-918.
3. Turakulov Jakhongir Ulugbekovich (2018). Complex compounds of calcium acetate with nitrocarbamide. Austrian Journal of Technical and Natural Sciences, (7-8), 67-72.
4. Turakulov, J. U. (2019). Synthesis, properties and application of new coordination compounds of calcium acetate with some amides, benzoic and nicotinic acids. diss. according to chem. Sciences.(PhD)-Tashkent.
5. Ibragimovna, Mukhamedova B., et al. "Quantitative Determination of the Preparation Cobalt-30 and Its Comparison of Leukopoesstimulating Effectiveness." *European Scholar Journal*, vol. 2, no. 3, 2021, pp. 71-73.
6. Mamatkulov M. et al. TECHNOLOGY FOR OBTAINING DIMETHYL ETHER //Science and Innovation. – 2022. – T. 1. – №. 5. – C. 125-129.
7. Narmatovich K. I. et al. Technology of Producing Dme //Academic Journal of Digital Economics and Stability. – 2021. – T. 9. – C. 127-133.